SURFACE REVERSIBLE MONOMERIZATION OF LIPOPHILIC REDOX PROTEINS-MATHCAD SIMULATIN PROTOCOL IN SQUARE-WAVE VOLTAMMETRY

Rubin Gulaboski

Faculty of Medical Sciences, Goce Delcev University, Stip, MACEDONIA

Abstract

The monomerization of lipophilic redox proteins on a surface can be reversible chemical process and it occurs when two identical small monomeric units react to form a larger, electrochemically active polymer. If the resulting structure can exchange electrons at the surface of the working electrode on which it is adsorbed, then the rate constant of monomerization, equilibrium constant of monomerization, and initial monomeric concentration can all affect the voltammetric outputs of the process. We have developed a theoretical model for simulating this complex electrode mechanism in square-wave voltammetry, and we are pleased to make the simulation protocol freely available to everyone.

$Es := 0.2$ $\Delta E := 0.8$ $dE := 0.004$ $Esw := 0.05$

$n := 1$ $F := 96500$ $R := 8.314$ $T := 298.15$

$j := 1..\frac{\Delta E}{dE}\cdot 50$

$\alpha := 0.5$

$pot_j := Es + Esw - \left[\left(ceil\left(\frac{j}{25}-\frac{1}{2}\right)\cdot dE + if\left(\frac{ceil\left(\frac{j}{25}\right)}{2} = ceil\left(\frac{j}{25}-\frac{1}{2}\right), 1, -1\right)\cdot Esw + Esw\right) - dE\right]$

$r := 1..1$ $cox := .075$ $2C > --Ox + 1e = \cdot Red$

$f := 10$

$ks_r := 10^{0.7\cdot r}$

$kf := .1$

$kb := .1$ $epsilon := kf + kb$

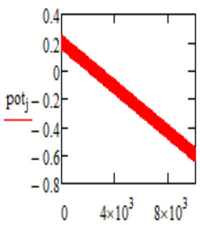
$\lambda_r := \frac{ks_r}{f}$ $K := 10^1$ $\lambda_r =$ 0.501 $\log\left(\frac{ks}{f_r}\right) =$

$\varepsilon := 10^1$ $\lambda_r =$ 0.501 $\varepsilon = 10$ $\varepsilon_r =$

$z := \frac{\varepsilon}{f}$

$\log(z_r) =$

$k := 1..\frac{\Delta E}{dE}\cdot 50$



$\frac{0.099}{0.119} = 0.832$

$\frac{.239}{.252} = 0.948$

$S_k := e^{\frac{z}{50}\cdot(-k)} - e^{\frac{z}{50}\cdot(-k+1)}$ $\varepsilon = 10$ $z = 1$

SURFACE MONOMERIZATION MECHANISM in SWV APRIL 2023

Kchem za monomerizacii e golemo treba vlijanie na cox i Keq i na KET

$10^{1.2} = 15.849$

$\log(z) = 0$

$\Phi_j := n\cdot\frac{F}{R\cdot T}\cdot pot_j$

$\varepsilon_r =$ $\log(\lambda_r) =$ -0.3

$\Psi =$

$$\Psi_{1,r} := \lambda_r \cdot e^{-\alpha\cdot\Phi_1} \cdot \frac{cox}{1+0} \cdot \left[(1)\cdot\left[\left[1 + \lambda_r \cdot e^{-\alpha\cdot\Phi_1} \cdot \frac{cox\cdot(K)}{(1+K)\cdot 50} - \frac{\lambda_r \cdot e^{-\alpha\cdot\Phi_1}\cdot S_1 \cdot cox}{(1+K)\cdot z}\right]\right]^2 + \frac{\lambda_r \cdot e^{(1-\alpha)\cdot\Phi_1}}{50}\right]^{-1}$$

$\Psi_{1,r} =$

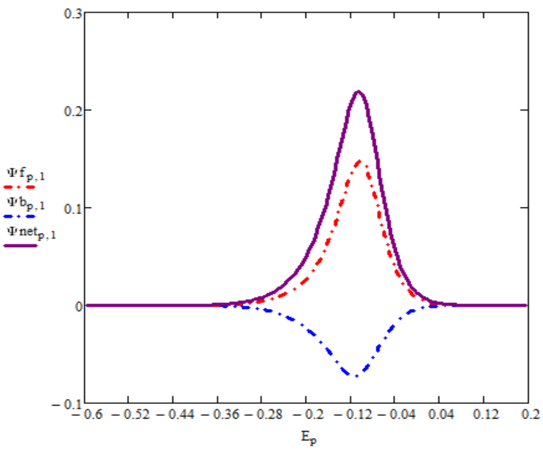
$$\Psi_{k,r} := \frac{\left[\left[\frac{\lambda_r \cdot e^{-\alpha\cdot\Phi_k}\cdot cox}{1+0}\cdot\left(1-\frac{1}{50}\cdot\sum_{j=1}^{k-1}\Psi_{j,r}\right) - \left[\frac{(z)^{-1}}{1+K}\cdot\lambda_r\cdot\left(\frac{cox}{1+0}\right)\cdot(-1)\cdot e^{-\alpha\cdot\Phi_k}\cdot\sum_{j=1}^{k-1}\left(\Psi_{j,r}\cdot S_{k-j+1}\right) - \frac{K}{1+K}\cdot\lambda_r\cdot\left(\frac{cox}{1+0}\right)\cdot(-1)\cdot e^{-\alpha\cdot\Phi_k}\cdot\sum_{j=1}^{k-1}\left(\Psi_{j,r}\cdot S_{k-j+1}\right)\right]\right]\right]^2 - \frac{\lambda_r}{50}\cdot e^{\Phi_k\cdot(1-\alpha)}\cdot\sum_{j=1}^{k-1}\Psi_{j,r}}{\left[\left(\frac{\lambda_r\cdot e^{-\alpha\cdot\Phi_k}\cdot 1}{1+0}\cdot\frac{cox}{50}\right) + 1 + \frac{(z)^{-1}}{1+K}\cdot\lambda_r\cdot(-1)\cdot\left(\frac{cox}{1+0}\right)\cdot S_1\cdot e^{-\alpha\cdot\Phi_k} + \frac{K}{1+K}\cdot\lambda_r\cdot(-1)\cdot\left(\frac{cox}{1+0}\right)\cdot S_1\cdot e^{-\alpha\cdot\Phi_k}\right]^2 + \frac{\lambda_r}{50}\cdot e^{\Phi_k\cdot(1-\alpha)}}$$

$p := 1..\left(\frac{\Delta E}{dE}\right) - 1$

$\Psi f_{p,r} := \Psi_{(p+1)\cdot 50,r}$ $\Psi b_{p,r} := \Psi_{50\cdot p+25}$ $\Psi net_{p,r} := \Psi f_{p,r} - \Psi b_{p,r}$

$E_p := Es - p \cdot dE$

$\exp\left(\frac{96480}{8.314\cdot 30}\right) = 9.833 \times 10^{167}$



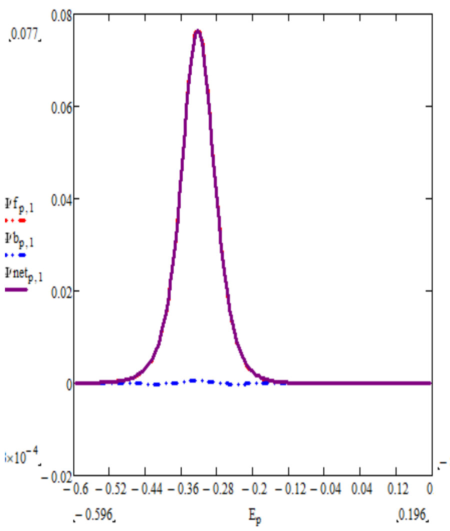
$K_{10} =$

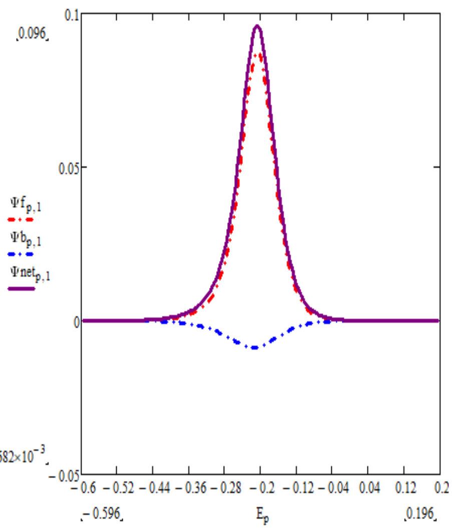
$E_p =$

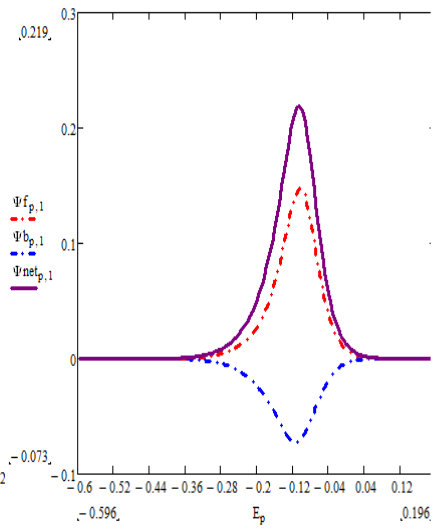
0.196
0.192
0.188
0.184
0.18
0.176
0.172
0.168
0.164

$\Psi f_{p,1} =$

9.08856·10-8
1.39981·10-7
2.11762·10-7
3.14969·10-7







Initial concentration changes from

0.00075; 0.0075; 0.075

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